Temperature inversion in granular fluids under gravity

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Abstract

We study, via hydrodynamic equations, the granular temperature profile of a granular fluid under gravity and subjected to energy injection from a base. It is found that there exists a turn-up in the granular temperature and that, far from the base, it increases linearly with height. We show that this phenomenon, observed previously in experiments and computer simulations, is a direct consequence of the heat flux law, different form Fourier's, in granular fluids. The positive granular temperature gradient is proportional to gravity and a transport coefficient μ_0, relating the heat flux to the density gradients, that is characteristic of granular systems. Our results provide a method to compute the value μ_0 for different restitution coefficients. The theoretical predictions are verified by means of molecular dynamics simulations, and the value of μ_0 is computed for the two dimensional inelastic hard sphere model. We provide, also, a boundary condition for the temperature field that is consistent with the modified Fourier's law.

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In a granular system a small amount of energy is lost at each collision between particles. This energy loss at the microscopic level leads to macroscopic dynamics quite different from those of systems with particles undergoing elastic collisions. One of the surprising consequences of the dissipative dynamics is the granular temperature inversion in fluidized granular systems under gravity. The granular temperature —the *temperature* from now on— is defined proportional to the mean kinetic energy per particle in the reference frame of the fluid. It has been observed that an open system subjected to a permanent energy injection from the base, exhibits a minimum of temperature at some distance from the boundary, and from there on temperature increases with height. In spite of the minimum the energy flux continues always pointing upwards. This fact confirms the existence of a heat flux law,

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different from Fourier's law, in these granular fluids. The heat flux is defined, for granular fluids, as the kinetic energy flux in the reference frame of the fluid. Nevertheless, the fact that the kinetic energy per particle, that is the granular temperature, can increase with increasing height from the base is unexpected, given the inelastic nature of collisions.

This temperature turn-up can be indirectly observed in experiments. For example, in [1] the authors report a temperature increase 30 times greater than expected due to the slow convective movement they observe in their experiments. Their conclusion is that this effect may not be attributed to convection currents, and suggest that it could be due to density gradients. The temperature minimum has also been observed in computer simulations [2,3] and a recent article accounts for this minimum with an hydrodynamic approach [4].

In this article, we deduce the presence of the minimum. Instead of solving the whole hydrodynamic equations for dilute granular gases as in [4], we show, using simple hydrodynamic arguments, that the temperature minimum has its origin in the modification of the Fourier law for the heat flux in granular fluids [5,6,7,8]. Also, unlike in [4], these simple hydrodynamic arguments predict, far from the base, a linear increase of temperature with height with a slope that can be deduced directly from the theory. This linear dependence is verified using molecular dynamic simulations of a simple granular model.

Consistently with these results, we establish the appropriate boundary condition for the temperature of an unbounded system, and for a system bounded by an upper adiabatic wall. Finally we provide a method to measure experimentally the transport coefficient associated with the non-Fourier heat flux law. All these results are compared with molecular dynamics simulations for a bi-dimensional system.

Hydrodynamic equations (that is, closed equations for a reduced number of macroscopic fields), resembling those of elastic systems, have been derived for the description of granular fluids [9,10,6]. Even though the validity of such description might be controversial [11,12], hydrodynamic equations together with appropriate constitutive relations have shown to be valid in quasi-elastic low-density stationary states.

The difference between the elastic and the granular hydrodynamic equations is an extra sink term in the energy balance equation which accounts for the energy dissipation. Also, constitutive relations are quite different in granular materials and in elastic systems. Fourier's Law, as mentioned, does not hold for these dissipative systems, but rather the heat flux follows a law in the form [5,6,7,8]

$$\mathbf{J} = -k\nabla T - \mu\nabla n, \tag{1}$$

$\mathbf{J}$ being the heat flux, k and μ the transport coefficients, T the granular temperature,

and n the number density. For small dissipation and low density, kinetic theory predicts that k and μ must be of the form

$$\begin{aligned} k &= k_0\sqrt{T}, \\ \mu &= \mu_0\frac{T^{3/2}}{n}, \end{aligned} \tag{2}$$

where k_0 and μ_0 depend only on the dissipative coefficient and μ_0 vanishes in the elastic limit. In quasi-elastic systems, $\mu_0 \ll k_0$ [8].

Experimentally, fluidized stationary states can be achieved by means of a vibrating base with some amplitude and frequency. In the low amplitude and high frequency limit, quasi-elastic systems reach non-equilibrium stationary states in which the vibrating base plays the role of a stationary boundary. A thermal wall is a useful theoretical model to describe this kind of boundary: each time a particle collides with the wall, it comes out with a velocity sorted out from a Maxwellian distribution.

While the results presented here should not depend on the particular mechanism of the energy injection, for simplicity, we will focus on an open system fluidized by a thermal base at the bottom. The system is kept bounded by a gravitational field pointing downwards with intensity g.

Such a system may exhibit different regimes. If density, gravity and dissipation are not too large, the system reaches a stationary state: the conductive regime. This state is characterized by a vanishing velocity field and density, temperature, and heat flux fields depending only on the vertical coordinate z. For increasing density, dissipation and/or gravity the system starts developing different instabilities such as Rayleigh Benard-like convection and solidification [13].

In the conductive regime, the energy dissipation at collisions induces a vertical temperature gradient. Energy is injected through the base and dissipated in the volume, with the corresponding decrease of the temperature with height. A snapshot of a typical configuration in the conductive regime is shown in Fig. 1.

Close to the base, we can state that the temperature decreases with height due to the high dissipation rate. Depending on the gravity acceleration and the inelasticity , the negative temperature gradient, is sometimes accompanied by a density increase which, at some extreme conditions, can lead to clustering and solidification.

Far from the base, on the other hand, we know that the density decreases by the action of gravity. Indeed, if the height is large enough ($z \geq 45$ in Fig. 1) we find just a few particles moving mainly in free flight, so that we can safely consider that there is a height above which the pressure is given by the ideal gas equation of state, $p = nT$.

The momentum balance equation states that the pressure obeys the barometric law $\frac{dp}{dz} = -ng$, so that together with the ideal gas expression for p we obtain,

$$n\frac{dT}{dz} + T\frac{dn}{dz} = -ng. \tag{3}$$

Inserting the expression for the density gradient derived from (3) into (1) and using the dilute limits for the transport coefficients (2), the heat flux far from the base is given by

$$J = -\left(k_0 - \mu_0\right)\sqrt{T}\frac{dT}{dz} + \mu_0 g\sqrt{T}. \tag{4}$$

As the density goes to zero with increasing height, the heat flux must consequently vanish as there are basically no particles to transport energy. It can be assumed then that there is a height where $J \ll \mu_0 g\sqrt{T}$. Above this height the heat flux in Eq. (4) can be neglected leading to the following relation for the temperature gradient as z goes to infinity

$$\frac{dT}{dz} = \frac{\mu_0 g}{k_0 - \mu_0}. \tag{5}$$

That is, the temperature gradient is a constant at high positions so that, far from the heating base, we can predict that the temperature field increases linearly with height with a slope proportional to g and μ_0.

Furthermore, as the temperature near the base decreases with height, it can be deduced, by continuity, that the temperature field has a minimum. Above the minimum, the temperature increases until it reaches the linear asymptotic dependence given by Eq. (5).

This prediction is fully corroborated in our MD simulations, as observed in Fig. 2 where the measured temperature profile has been plotted for two different systems. In both of them we clearly observe the minimum and the further linear increase of the temperature.

In our MD simulations, the inelastic hard sphere model (IHS) in two dimensions is used as the microscopic model for the particles. Grains are modeled as smooth hard disks that dissipate energy at each collision through a constant dissipative coefficient q, related to the normal restitution coefficient $r = 1 - 2q$, so that $q = 0$ represents the elastic case. The simulated systems are composed of N inelastic hard disks. In the horizontal direction x, we set periodic boundary conditions. The box width is L. At the bottom we imposed a thermal wall at temperature T_0. Due to the absence of an intrinsic energy scale in the IHS model, we fix the temperature T_0

to unity. Results for other temperatures are obtained by simple dimensional analysis. Also, units are chosen such that the disks diameters σ and masses m are set to one. In these units the dimensionless gravity is $\hat{g} = mg\sigma/T_0$. The system is completely defined giving the values of N, L, $\hat{g}$, and the dissipative coefficient q. For each value of the parameters we thermalize the system after which we measure the macroscopic fields, averaging over a long simulation time.

In Fig. 2 we present the results for: system A (dashed line) with parameters $N = 1120$, $L = 89.44$, $q = 0.01$, and $\hat{g} = 0.02$; and system B (solid curve) with $N = 560$, $L = 44.72$, $q = 0.01$, and $\hat{g} = 0.03$. The snapshot presented in Fig. 1 corresponds to the system A. Comparing both figures it can be observed that the temperature minimum (at $z \approx 45\sigma$) lies close to the free surface of the system but still into the bulk. The system size, under which 99% of the particles lie, is 60σ so that the observed linear dependence of the temperature remains up to twice the system size, proving to be the real asymptotic behavior. Similar behavior is observed in system B, that has an effective height of $z = 45\sigma$ and the temperature minimum is located at $z = 35\sigma$. For higher positions, the density is very low implying large statistical errors.

To test any possible finite size dependence on the temperature slope, we performed simulations for different number of particles N, keeping fixed the ratio N/L. We found that even if the profiles $n(z)$ and $T(z)$ may suffer variations, the asymptotic temperature slope remains independent of N for $N \geq 280$.

We could deduce from these results that the temperature could achieve arbitrarily large values as height increases. However, our hydrodynamic description is limited because of the zero density, or infinite Knudsen number, limit at these heights. Our prediction at high positions is, nevertheless, physically meaningful as the combined effect of the temperature increase (linear) and the density decrease (almost exponential) is a net decrease of the energy density with height. So, even if the average kinetic energy per particle increases, the total energy of the system remains always finite. In summary, the prediction of the linear regime is valid up to some height after which the starting equations (hydrodynamics) are not valid, but anyway give physically meaningful predictions.

A system bounded by an upper adiabatic wall (that is, grains are reflected elasticaly) is a similar, although not identical, problem to that of the unbounded system. At an adiabatic boundary, the heat flux is exactly zero so that Eq. (5) is the exact expression for the temperature gradient at the wall if the density at the wall is low enough. The temperature gradient at the elastic wall is then positive, provided $\mu_0 \ll k_0$. This ensures the existence of a minimum, as the temperature gradient is negative at the base. The minimum of temperature induced by an upper elastic wall has been observed in one dimensional simulations [14].

It is clear that these results concern closely the boundary condition for the tem-

perature field that must be used to solve the hydrodynamic equations in granular systems. In an unbounded system under gravity, Eq. (5) must be imposed as the boundary condition for the temperature at infinity. The same boundary condition applies to any adiabatic wall, contrary to the usual condition $dT/dz = 0$ that has traditionally been used in computations of granular systems.

Those experiments where the stationary temperature inversion has been observed [1], have the normal lack of statistics at high positions and the linear increase of temperature can not be easily detected, specially if this is not the final purpose of the experiment. We want to stress that the measurement of the temperature slope, either experimentally or in simulations, provides a method to obtain the transport coefficient μ_0 for small dissipation coefficients.

As an example, we have calculated the value of μ_0, at the lowest order in the dissipative coefficient q, for the two dimensional inelastic hard sphere model. We consider systems with $N = 560$ and $L = 44.72$. In order to avoid instabilities –especially the convection described in Ref. [13]– systems with low dissipative coefficients and low gravity values have to be considered. Our simulations have been done with $\hat{g} = 0.01$ and $\hat{g} = 0.02$, and $0.002 \leq q \leq 0.02$.

For these small values of q, we can use $(k_0 - \mu_0) \approx k_0$ to first order in q . Also, in the same order of approximation, k_0 can be set to that of the elastic hard disk system, $k_0 = 2/\sqrt{\pi}$, neglecting the linear correction in q. Then, μ_0 is given by

$$\mu_0 = \frac{2}{\sqrt{\pi} g} \frac{dT}{dy}, \tag{6}$$

expression that is valid only up to order q.

In Fig. 3, we present results for μ_0 obtained in the simulations. It can be observed that the two sets, with different values of $\hat{g}$, collapse into the same curve, confirming the linearity with $\hat{g}$ of the temperature gradient.

As expected, μ_0 goes to zero in the elastic limit. The computed values of the two series are fitted to a single quadratic function in q where it is imposed that μ_0 must vanish for $q = 0$. The obtained fit is

$$\mu_0 = 0.64q + 106q^2 \tag{7}$$

noting that only the linear term in the last fit is consistent with the approximation done. In Ref. [8] the authors computed μ_0 using a different method from that described in here, with the result $\mu_0 = 0.7q$ which agrees with the result found in the present paper. Nevertheless, we want to point out that the present method for computing μ_0 uses the temperature profile over a wide range (the region where T

increases linearly) instead of using the information over just one point as in Ref. [8]. Therefore this method of computing μ_0 is more accurate in the dilute case.

In the highly fluidized regime, the particular energy injection mechanism becomes irrelevant far from the energetic boundary. This implies that even in a system on a vibrating base, the method presented here should be fully valid. Also, even though our predictions are valid in the dilute case, we expect that in denser regimes there should be also a temperature turn-up and a temperature increase with height (though maybe not linear). In this case, there are explicit density dependences in the equation of state and transport coefficients, giving rise to a more complex differential equation for T compared to (5). Nevertheless, as long as there is a non-vanishing coefficient μ, the equation is not trivial and a temperature gradient is predicted.

In summary, we have shown that the granular temperature turn-up observed in vibrofluidized granular systems has its origin in the modification of the Fourier law for the granular heat flux. The vanishing energy flux far from the base together with the density gradient produced by the gravity imposes a positive and constant temperature gradient. Careful measurements of this gradient provide a method to compute the transport coefficient μ_0, either experimentally or in simulations.

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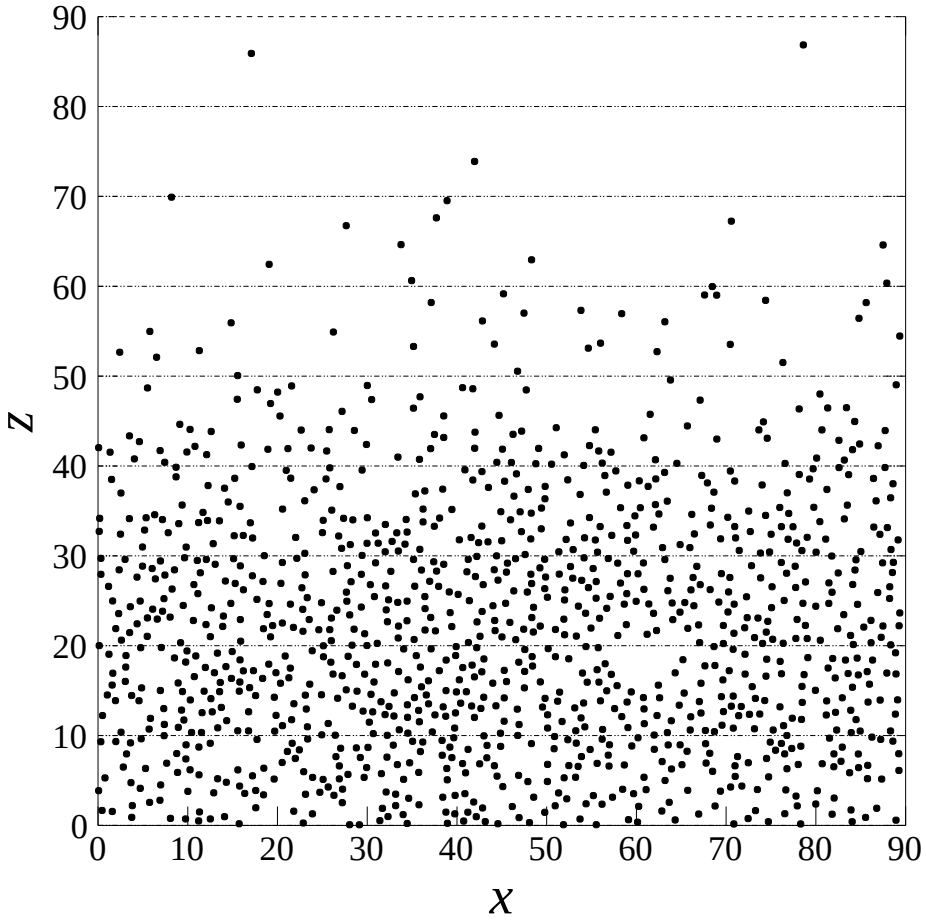

Fig. 1. Snapshot of an open granular system obtained in a bi-dimensional molecular dynamics simulations of the inelastic hard sphere model. The system is fluidized by a thermal injection base and it is kept bounded by the gravity field pointing downwards.

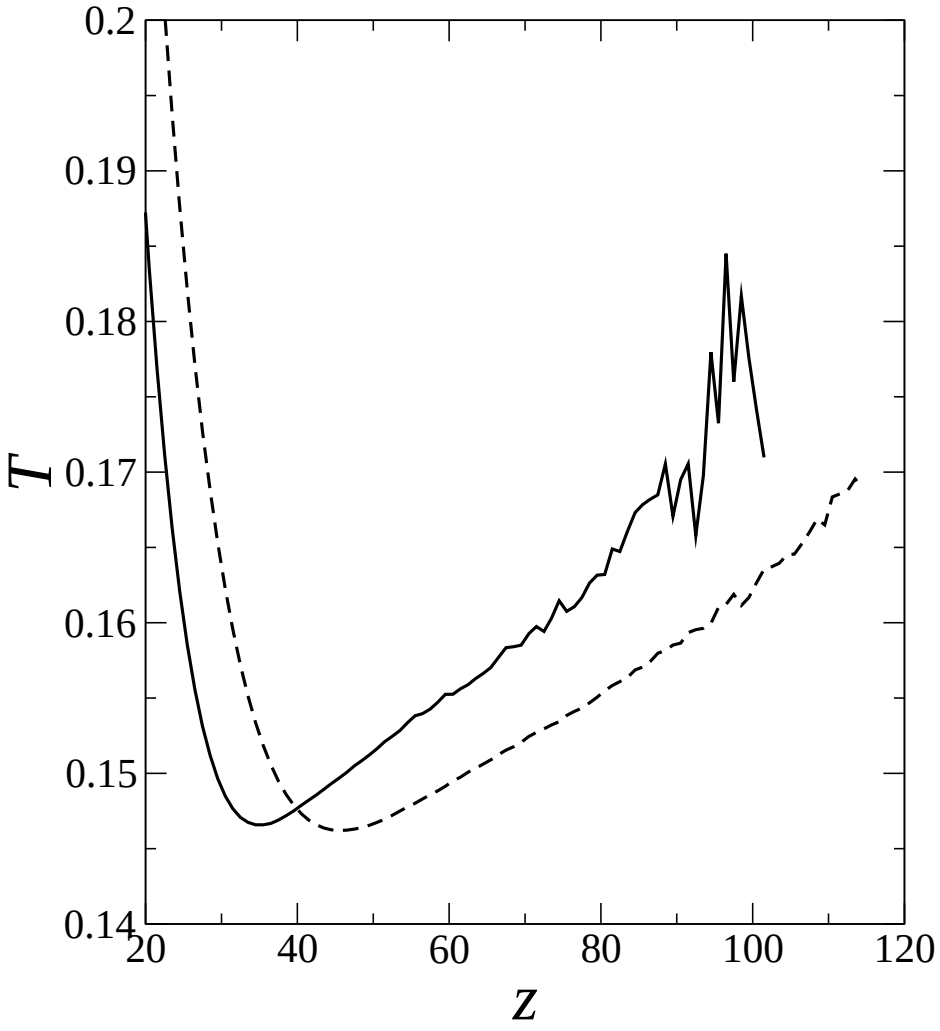

Fig. 2. Temperature profile obtained from MD simulations. System A (dashed curve) corresponds to $N = 1120$, $L = 89.44$, $q = 0.01$, and $\hat{g} = 0.02$. System B (solid curve) corresponds to $N = 560$, $L = 44.72$, $q = 0.01$, and $\hat{g} = 0.03$.

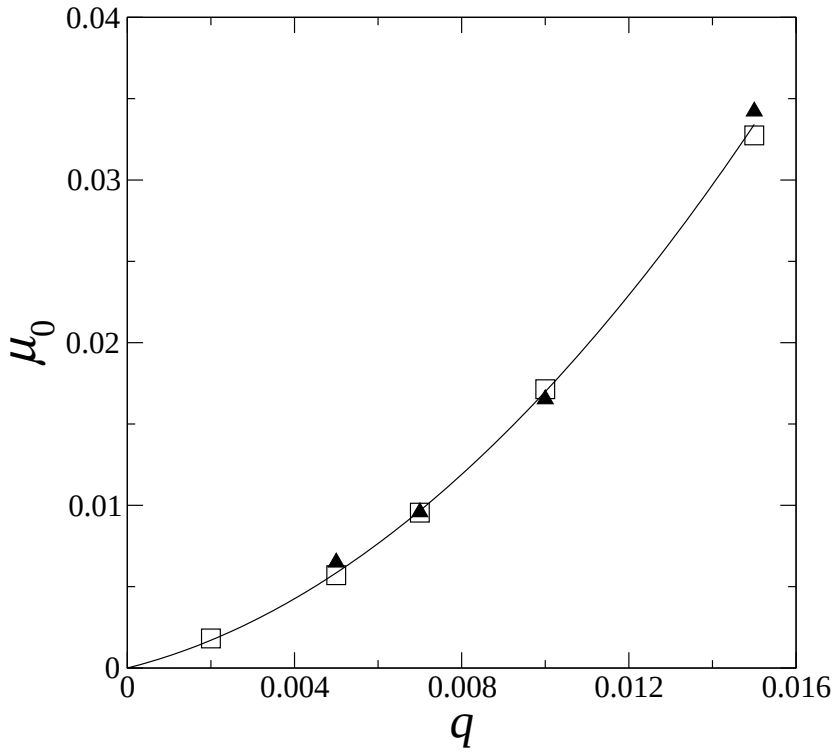

Fig. 3. Computed values of μ_0 as a function of q obtained in two series of simulations. Solid triangles correspond to $\hat{g} = 0.01$ and open squares to $\hat{g} = 0.02$. The solid curve is a quadratic fit in q of the obtained data.